Table 14. Anisotropic displacement parameters ($Å^2 x 10^4$) for 5 CCDC 147897 pjc20. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
ZrA	160(3)	199(6)	143(3)	-1(5)	35(2)	4(5)
ZrB	149(3)	180(5)	150(3)	12(5)	30(2)	-14(5)
Si1	176(3)	257(3)	185(3)	8(2)	68(2)	1(2)
Si2	258(3)	208(3)	232(3)	14(2)	53(2)	27(2)
Si3	206(3)	227(3)	205(3)	18(2)	45(2)	-3(2)
N1	347(14)	245(14)	249(13)	0	124(11)	0
N2	182(12)	245(14)	414(15)	0	40(11)	0
C1	205(10)	263(11)	134(9)	4(8)	49(8)	4(8)
C2	226(10)	216(10)	173(9)	-27(8)	35(8)	18(8)
C3	180(10)	260(11)	151(9)	7(8)	13(8)	35(9)
C4	197(10)	272(11)	159(9)	39(8)	37(8)	7(8)
C5	182(10)	276(12)	257(11)	98(9)	40(8)	43(9)
C6	133(9)	235(10)	193(10)	-1(8)	35(7)	-12(8)
C7	255(11)	242(11)	246(11)	65(9)	123(9)	70(9)
C8	167(9)	277(11)	218(10)	6(8)	52(8)	27(8)
C9	168(9)	282(11)	150(9)	-6(8)	16(8)	-28(8)
C10	197(10)	228(10)	189(10)	-19(8)	28(8)	-27(8)
C11	229(11)	331(13)	234(11)	-21(10)	74(9)	13(10)
C12	240(11)	331(13)	247(12)	40(10)	88(10)	-25(10)
C13	352(14)	302(14)	286(12)	36(11)	64(10)	25(11)
C14	317(12)	350(14)	241(11)	42(11)	54(10)	43(11)
C15	358(14)	253(13)	382(14)	-2(11)	99(12)	30(11)
C16	183(9)	252(11)	254(10)	52(9)	49(8)	2(8)
C17	222(11)	290(13)	315(12)	-22(10)	91(10)	-50(10)
C18	341(13)	261(13)	383(14)	-13(11)	149(11)	-8(11)
C19	261(13)	372(15)	459(16)	189(13)	22(11)	-45(11)
C20	294(11)	274(12)	298(11)	2(9)	142(9)	64(9)
C21	1170(40)	610(20)	491(19)	138(18)	370(20)	670(30)
C22	413(16)	329(16)	910(30)	-260(17)	295(17)	-87(13)
C23	410(15)	407(16)	423(15)	-157(13)	276(13)	-70(13)
C24	310(13)	239(12)	326(13)	41(10)	24(10)	4(10)
C25	256(11)	261(13)	284(12)	24(10)	69(9)	15(10)
C26	199(11)	408(15)	247(11)	73(11)	37(9)	20(11)
C27	364(19)	268(18)	398(19)	0	42(15)	0
C28	261(12)	399(15)	349(13)	-62(11)	56(10)	-118(11)
C29	226(11)	392(14)	291(12)	-71(10)	62(9)	23(10)
C30	273(15)	308(17)	159(13)	0	15(12)	0
C31	460(20)	360(20)	330(20)	0	107(19)	0

Table 15. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for 5 CCDC 147897 pjc20.

	x	y	z	U_{iso}
H3	220(1)	134(2)	55(1)	19(5)
H5	425(1)	-70(2)	126(1)	28(6)
H7	468(1)	380(2)	199(1)	23(6)
H9	443(1)	167(2)	373(1)	19(5)
H11A	647(1)	53(2)	133(1)	36(6)
H11B	587(1)	9(2)	61(1)	31(6)
H11C	582(1)	-38(2)	137(1)	33(7)
H12A	616(1)	319(2)	113(1)	24(5)
H12B	528(2)	369(2)	79(1)	50(8)
H12C	570(1)	288(2)	33(1)	25(5)
H13A	381(2)	387(2)	-99(1)	46(7)
H13B	388(2)	252(3)	-95(2)	57(8)
H13C	451(2)	334(2)	-47(1)	39(7)
H14A	214(1)	408(2)	-81(1)	39(6)
H14B	186(1)	335(2)	-17(1)	32(6)
H14C	214(1)	258(2)	-80(1)	42(7)
H15A	336(1)	550(2)	21(1)	45(7)
H15B	403(2)	494(2)	77(1)	43(7)
H15C	318(2)	493(2)	90(2)	49(8)
H17A	169(1)	-65(2)	158(1)	35(6)
H17B	138(1)	-176(2)	105(1)	14(5)
H17C	139(1)	-36(2)	76(1)	27(6)
H18A	220(1)	-128(2)	-21(1)	39(6)
H18B	216(1)	-257(2)	18(1)	36(6)
H18C	295(2)	-206(2)	6(1)	37(7)
H19A	303(1)	-186(2)	200(1)	39(7)
H19B	351(2)	-243(2)	147(1)	39(7)
H19C	264(1)	-291(2)	155(1)	31(6)
H21A	325(2)	491(4)	255(2)	108(19)
H21B	402(2)	550(3)	247(2)	70(10)
H21C	357(2)	597(3)	304(2)	62(8)
H22A	521(2)	435(2)	411(1)	47(8)
H22B	478(2)	564(2)	401(1)	50(7)
H22C	524(2)	510(3)	341(2)	70(9)
H23A	313(2)	357(2)	365(1)	46(7)
H23B	349(1)	466(2)	415(1)	43(7)
H23C	388(2)	338(3)	429(2)	81(11)
H24A	466(1)	-191(2)	272(1)	29(6)
H24B	553(1)	-239(2)	296(1)	33(6)
H24C	527(1)	-175(2)	221(1)	43(7)
H25A	696(2)	-49(2)	343(1)	50(7)
H25B	678(1)	89(2)	335(1)	35(6)
H25C	673(1)	11(2)	264(1)	37(6)
H26A	495(1)	-61(2)	423(1)	33(6)
H26B	566(1)	27(2)	444(1)	38(7)
H26C	580(1)	-110(2)	440(1)	43(7)

H27[a]	750	221(3)	250	26(8)
H28	648(1)	334(2)	289(1)	32(6)
H29	646(1)	545(2)	284(1)	32(6)
H31A[a]	810(3)	743(4)	251(3)	30(12)
H31B[a]	736(3)	733(4)	296(3)	22(11)
H31C[a]	710(4)	742(4)	205(3)	39(14)

[a] Population: ½

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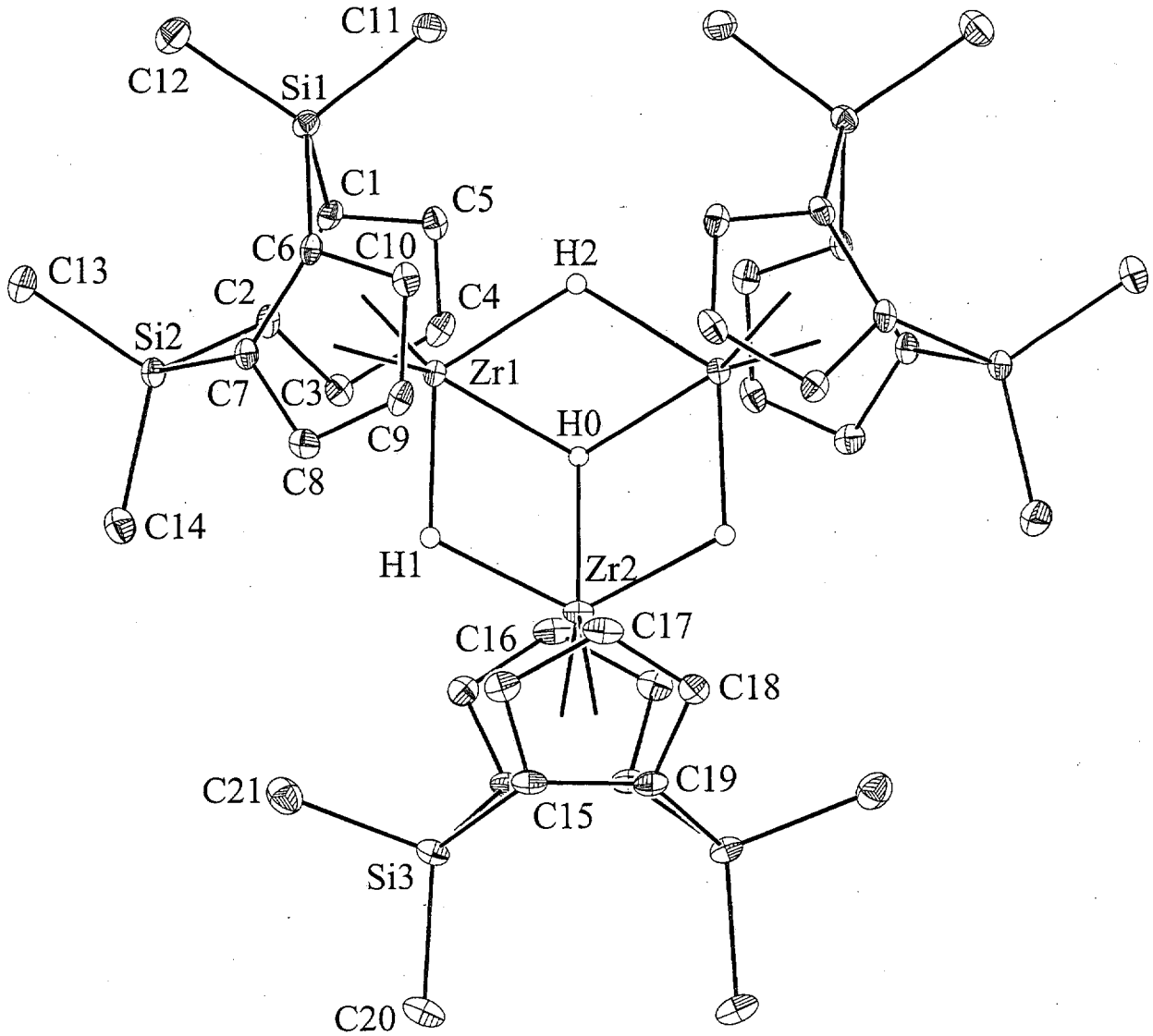
Principal mean square atomic displacements U

0.0200	0.0161	0.0139	ZrA
0.0190	0.0152	0.0137	ZrB
0.0258	0.0209	0.0138	Si1
0.0271	0.0229	0.0195	Si2
0.0237	0.0209	0.0189	Si3
0.0371	0.0245	0.0199	N1
0.0420	0.0245	0.0182	N2
0.0264	0.0206	0.0126	C1
0.0249	0.0209	0.0158	C2
0.0274	0.0182	0.0142	C3
0.0284	0.0196	0.0145	C4
0.0365	0.0198	0.0151	C5
0.0236	0.0193	0.0130	C6
0.0373	0.0183	0.0156	C7
0.0284	0.0219	0.0154	C8
0.0288	0.0174	0.0142	C9
0.0245	0.0201	0.0171	C10
0.0336	0.0257	0.0189	C11
0.0349	0.0278	0.0175	C12
0.0364	0.0317	0.0257	C13
0.0385	0.0297	0.0227	C14
0.0399	0.0339	0.0243	C15
0.0305	0.0202	0.0178	C16
0.0348	0.0281	0.0182	C17
0.0435	0.0262	0.0258	C18
0.0638	0.0262	0.0209	C19
0.0386	0.0280	0.0166	C20
0.1630	0.0415	0.0143	C21
0.1035	0.0322	0.0229	C22
0.0671	0.0342	0.0151	C23
0.0370	0.0297	0.0221	C24
0.0306	0.0246	0.0242	C25
0.0436	0.0224	0.0196	C26
0.0422	0.0351	0.0268	C27
0.0479	0.0338	0.0193	C28
0.0432	0.0265	0.0205	C29
0.0308	0.0284	0.0157	C30
0.0462	0.0355	0.0311	C31



11 CCDC 110868 pjc6

Table 16. Crystal data and structure refinement for 11 CCDC 110868 PJC6.

Empirical formula	$C_{42}H_{59}Si_6Zr_3$
Formula weight	1006.11
Crystallization Solvent	C_6D_6
Crystal Habit	Prism
Crystal size	0.52 x 0.26 x 0.10 mm^3
Crystal color	Dichroic, dark brown-green / colorless

Data Collection

Preliminary Photos	None	
Type of diffractometer	CAD-4	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	84 K	
Theta range for reflections used in lattice determination	15 to 17°	
Unit cell dimensions	a = 15.804(4) Å	α= 90°
	b = 15.804(4) Å	β= 90°
	c = 17.018(3) Å	γ = 90°
Volume	4250.5(17) $Å^3$	
Z	4	
Crystal system	Tetragonal	
Space group	$P4_32_12$ (#96)	
Density (calculated)	1.572 Mg/m^3	
F(000)	2060	
Theta range for data collection	1.5 to 25°	
Completeness to theta = 25°	100.0 %	
Index ranges	0<=h<=18, -18<=k<=18, 0<=l<=20	
Data collection scan type	Ω–scans	
Reflections collected	13292	
Independent reflections	3746 [R_{int}= 0.021; GOF_{merge}= 1.11]	
Absorption coefficient	0.921 mm^{-1}	
Absorption correction	None	
Number of standards	3 reflections measured every 75 min.	
Variation of standards	0%, within experimental error	

Table 16 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	difference map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3746 / 0 / 349
Treatment of hydrogen atoms	all parameters refined
Goodness-of-fit on F^2	1.627
Final R indices [$I>2\sigma(I)$]	R1 = 0.0163, wR2 = 0.0403
R indices (all data)	R1 = 0.0168, wR2 = 0.0405
Type of weighting scheme used	calculated
Weighting scheme used	$w=1/\sigma^2(F_o^2)$
Max shift/error	0.043
Average shift/error	0.002
Absolute structure parameter	0.00(2)
Largest diff. peak and hole	0.252 and -0.308 e.Å^{-3}

Special Refinement Details

Data were collected with 1° ω-scans.

The individual backgrounds were replaced by a background function of 2θ derived from those reflections with $I < 8\sigma(I)$.

The GOF_{merge} was 1.11 (3743 multiples).

The molecule lies on a 2-fold axis through Zr2 and H2. For all molecules, the plane through the three Zr atoms is almost perpendicular to the c-axis.

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$, variances of the merged data were obtained by propagation of error plus another additional term, $(0.014<I>)^2$.

N.B. CpnC refers to centroid n; CpnP refers to plane n.

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 11 CCDC 110868 PJC6A. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Zr1	6692(1)	4803(1)	2461(1)	8(1)
Zr2	4688(1)	5312(1)	2500	9(1)
Si1	8670(1)	4171(1)	2608(1)	11(1)
Si2	8175(1)	6250(1)	2205(1)	11(1)
Si3	4211(1)	7343(1)	2564(1)	12(1)
C1	8038(1)	4497(1)	1721(1)	11(1)
C2	7809(1)	5366(1)	1558(1)	10(1)
C3	7063(1)	5343(1)	1083(1)	11(1)
C4	6839(1)	4492(1)	946(1)	12(1)
C5	7428(1)	3979(1)	1338(1)	12(1)
C6	8015(1)	4829(1)	3289(1)	10(1)
C7	7810(1)	5702(1)	3125(1)	10(1)
C8	7053(1)	5888(1)	3542(1)	12(1)
C9	6796(1)	5162(1)	3964(1)	12(1)
C10	7374(1)	4510(1)	3805(1)	12(1)
C11	8524(2)	3035(1)	2863(1)	15(1)
C12	9831(2)	4397(2)	2606(2)	19(1)
C13	9329(1)	6478(2)	2102(1)	15(1)
C14	7549(2)	7228(1)	2033(2)	17(1)
C15	4086(1)	6496(1)	3326(1)	12(1)
C16	4746(2)	6149(1)	3796(1)	13(1)
C17	4509(1)	5334(1)	4039(1)	13(1)
C18	3711(1)	5156(2)	3719(1)	12(1)
C19	3429(1)	5864(1)	3271(1)	12(1)
C20	3432(2)	8228(1)	2618(2)	20(1)
C21	5288(2)	7819(2)	2593(2)	19(1)

Table 18. Distances [Å] and angles [°] for 11 CCDC 110868 PJC6.

Zr1-Cp1C[1]	2.2593	C5-H5	0.97(2)
Zr1-Cp2C	2.2622	C6-C10	1.432(3)
Zr1-Cp1P[2]	2.2543(11)	C6-C7	1.444(3)
Zr1-Cp2P	2.2591(11)	C7-C8	1.422(3)
Zr1-Zr2	3.2687(9)	C8-C9	1.412(3)
Zr1-Zr1^{i}	3.3443(9)	C8-H8	0.91(2)
Zr1-H0	2.17(2)	C9-C10	1.404(3)
Zr1-H1	1.93(2)	C9-H9	0.95(3)
Zr1-H2	1.96(1)	C10-H10	0.95(2)
H0-H0^{i}	1.85(4)	C11-H11A	0.86(2)
Zr1-C1	2.520(2)	C11-H11B	0.94(3)
Zr1-C2	2.504(2)	C11-H11C	0.91(3)
Zr1-C3	2.564(2)	C12-H12A	0.92(3)
Zr1-C4	2.635(2)	C12-H12B	0.83(3)
Zr1-C5	2.589(2)	C12-H12C	0.85(3)
Zr1-C6	2.521(2)	C13-H13A	0.93(3)
Zr1-C7	2.532(2)	C13-H13B	1.00(3)
Zr1-C8	2.578(2)	C13-H13C	0.85(3)
Zr1-C9	2.625(2)	C14-H14A	0.88(3)
Zr1-C10	2.570(2)	C14-H14B	0.88(3)
Zr2-Cp3C	2.2726	C14-H14C	0.92(3)
Zr2-Cp3P	2.2690(10)	C15-C16	1.425(3)
Zr2-Zr1^{i}	3.2687(9)	C15-C19	1.443(3)
Zr2-H0	2.04(2)	C16-C17	1.404(3)
Zr2-H1	1.95(2)	C16-H16	0.94(2)
Zr2-C15	2.525(2)	C17-C18	1.401(3)
Zr2-C16	2.573(2)	C17-H17	0.89(2)
Zr2-C17	2.634(2)	C18-C19	1.426(3)
Zr2-C18	2.597(2)	C18-H18	0.90(2)
Zr2-C19	2.537(2)	C19-Si3^{i}	1.877(2)
Si1-C11	1.862(2)	C20-H20A	0.88(3)
Si1-C12	1.869(2)	C20-H20B	0.90(3)
Si1-C6	1.871(2)	C20-H20C	0.92(3)
Si1-C1	1.882(2)	C21-H21A	0.87(3)
Si2-C14	1.858(2)	C21-H21B	0.95(3)
Si2-C13	1.868(2)	C21-H21C	1.00(3)
Si2-C2	1.871(2)		
Si2-C7	1.879(2)	Cp1C-Zr1-Cp2C	116.63
Si3-C21	1.862(2)	Cp1C-Zr1-Zr2	122.22
Si3-C20	1.865(2)	Cp2C-Zr1-Zr2	113.45
Si3-C15	1.873(2)	Cp1C-Zr1-Zr1^{i}	111.57
Si3-C19^{i}	1.877(2)	Cp2C-Zr1-Zr1^{i}	121.78
C1-C5	1.422(3)	Zr2-Zr1-Zr1^{i}	59.232(4)
C1-C2	1.447(3)	Cp1C-Zr1-H0	96.4
C2-C3	1.431(3)	Cp2C-Zr1-H0	146.8
C3-C4	1.410(3)	Zr2-Zr1-H0	37.6(6)
C3-H3	0.88(2)	Zr1^{i}-Zr1-H0	38.8(6)
C4-C5	1.402(3)	Cp1C-Zr1-H1	110.0
C4-H4	0.83(2)	Cp2C-Zr1-H1	100.3

Zr2-Zr1-H1	32.8(6)
$Zr1^{i}$-Zr1-H1	91.9(6)
H0-Zr1-H1	63.0(8)
Cp1C-Zr1-H2	95.9
Cp2C-Zr1-H2	111.7
Zr2-Zr1-H2	90.8(7)
$Zr1^{i}$-Zr1-H2	31.6(7)
H0-Zr1-H2	64.9(8)
H1-Zr1-H2	123.5(9)
Cp1P-Cp2P	70.12(6)
Cp3C-Zr2-$Zr1^{i}$	114.35
Cp3C-Zr2-Zr1	119.93
$Zr1^{i}$-Zr2-Zr1	61.536(8)
Cp3C-Zr2-H0	148.8
$Zr1^{i}$-Zr2-H0	39.6(7)
Zr1-Zr2-H0	40.5(7)
Cp3C-Zr2-H1	111.2
$Zr1^{i}$-Zr2-H1	93.7(6)
Zr1-Zr2-H1	32.3(6)
H0-Zr2-H1	65.1(10)
$Cp3P^{i}$-Cp3P	70.46(6)
C11-Si1-C12	107.82(11)
C11-Si1-C6	108.87(10)
C12-Si1-C6	116.01(10)
C11-Si1-C1	112.66(10)
C12-Si1-C1	117.83(11)
C6-Si1-C1	92.95(9)
C14-Si2-C13	110.17(11)
C14-Si2-C2	111.37(11)
C13-Si2-C2	112.94(10)
C14-Si2-C7	110.60(10)
C13-Si2-C7	117.83(10)
C2-Si2-C7	92.91(9)
C21-Si3-C20	107.35(11)
C21-Si3-C15	111.48(10)
C20-Si3-C15	115.63(11)
$C21-Si3-C19^{i}$	109.93(11)
$C20-Si3-C19^{i}$	118.91(11)
$C15-Si3-C19^{i}$	93.04(9)
C5-C1-C2	106.76(18)
C5-C1-Si1	124.75(16)
C2-C1-Si1	123.07(15)
C3-C2-C1	106.87(18)
C3-C2-Si2	127.32(16)
C1-C2-Si2	121.29(15)
C4-C3-C2	108.91(19)
C4-C3-H3	129.4(14)
C2-C3-H3	121.7(14)
C5-C4-C3	107.82(19)
C5-C4-H4	126.2(17)
C3-C4-H4	125.9(17)
C4-C5-C1	109.64(19)
C4-C5-H5	127.0(12)
C1-C5-H5	123.4(12)
C10-C6-C7	107.25(18)
C10-C6-Si1	125.13(16)
C7-C6-Si1	122.37(15)
C8-C7-C6	106.81(18)
C8-C7-Si2	125.38(16)
C6-C7-Si2	122.19(15)
C9-C8-C7	109.14(19)
C9-C8-H8	127.4(14)
C7-C8-H8	123.5(14)
C10-C9-C8	108.14(19)
C10-C9-H9	127.9(15)
C8-C9-H9	123.9(15)
C9-C10-C6	108.64(18)
C9-C10-H10	122.7(14)
C6-C10-H10	128.7(14)
Si1-C11-H11A	111.7(15)
Si1-C11-H11B	109.0(17)
H11A-C11-H11B	100(2)
Si1-C11-H11C	110.0(17)
H11A-C11-H11C	117(2)
H11B-C11-H11C	108(2)
Si1-C12-H12A	110.8(18)
Si1-C12-H12B	113(2)
H12A-C12-H12B	107(3)
Si1-C12-H12C	111(2)
H12A-C12-H12C	108(3)
H12B-C12-H12C	106(3)
Si2-C13-H13A	112.0(18)
Si2-C13-H13B	109.9(15)
H13A-C13-H13B	104(2)
Si2-C13-H13C	111.1(17)
H13A-C13-H13C	114(2)
H13B-C13-H13C	106(2)
Si2-C14-H14A	110(2)
Si2-C14-H14B	109.4(17)
H14A-C14-H14B	104(2)
Si2-C14-H14C	114(2)
H14A-C14-H14C	118(3)

H14B-C14-H14C	101(2)	C18-C19-Si3^{i}	123.93(17)
C16-C15-C19	107.2(2)	C15-C19-Si3^{i}	124.05(17)
C16-C15-Si3	125.97(17)	Si3-C20-H20A	108.7(17)
C19-C15-Si3	121.67(17)	Si3-C20-H20B	114.4(19)
C17-C16-C15	108.9(2)	H20A-C20-H20B	108(3)
C17-C16-H16	125.6(14)	Si3-C20-H20C	108.7(17)
C15-C16-H16	125.6(14)	H20A-C20-H20C	99(2)
C18-C17-C16	108.08(18)	H20B-C20-H20C	117(3)
C18-C17-H17	125.6(12)	Si3-C21-H21A	112.9(19)
C16-C17-H17	126.3(12)	Si3-C21-H21B	109.3(16)
C17-C18-C19	109.3(2)	H21A-C21-H21B	111(2)
C17-C18-H18	125.6(14)	Si3-C21-H21C	109.7(15)
C19-C18-H18	125.0(14)	H21A-C21-H21C	108(2)
C18-C19-C15	106.5(2)	H21B-C21-H21C	106(2)

Symmetry transformations used to generate equivalent atoms:
^{i} -y+1,-x+1,-z+1/2

[1] Cp1C is the centroid of atoms C1,C2,C3,C4,C5
Cp2C is the centroid of atoms C6,C7,C8,C9,C10
Cp3C is the centroid of atoms C15,C16,C17,C18,C19

[2] Cp1P is the best plane through atoms C1,C2,C3,C4,C5
Cp2P is the best plane through atoms C6,C7,C8,C9,C10
Cp3P is the best plane through atoms C15,C16,C17,C18,C19

Table 19. Anisotropic displacement parameters ($Å^2 x 10^4$) for 11 CCDC 110868 PJC6. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr1	84(1)	95(1)	60(1)	3(1)	-3(1)	-13(1)
Zr2	105(1)	105(1)	55(1)	0(1)	0(1)	31(1)
Si1	89(3)	122(3)	106(3)	-9(2)	-11(2)	0(2)
Si2	112(3)	107(3)	97(3)	3(2)	7(2)	-22(2)
Si3	152(3)	100(3)	108(3)	6(3)	-6(3)	31(2)
C1	86(10)	141(11)	88(10)	-10(8)	37(8)	-12(8)
C2	113(10)	121(10)	71(9)	22(8)	44(8)	-38(9)
C3	140(11)	116(11)	66(10)	27(9)	26(8)	-12(9)
C4	99(11)	198(11)	54(10)	-10(9)	22(9)	-19(9)
C5	140(11)	119(11)	89(10)	-14(8)	43(9)	-33(8)
C6	86(10)	118(10)	82(9)	-12(8)	-29(8)	-34(8)
C7	108(10)	110(10)	78(10)	-16(8)	-27(8)	-31(8)
C8	151(11)	120(11)	93(10)	-51(9)	-35(9)	-2(9)
C9	103(10)	169(11)	76(10)	-45(9)	-3(8)	-41(9)
C10	142(11)	135(11)	69(9)	7(9)	-45(8)	-31(9)
C11	153(12)	139(11)	170(12)	-4(10)	-8(10)	20(9)
C12	133(11)	229(13)	214(13)	-17(11)	-7(11)	-5(10)
C13	127(11)	185(12)	142(11)	-3(10)	13(10)	-39(9)
C14	191(12)	146(11)	180(12)	19(10)	1(10)	-24(10)
C19	120(11)	144(11)	96(10)	-16(9)	35(9)	44(9)
C15	143(11)	128(11)	83(10)	-41(9)	21(8)	52(9)
C16	153(12)	171(11)	66(10)	-41(9)	16(9)	26(10)
C17	183(11)	159(12)	39(9)	-7(9)	22(8)	76(9)
C18	145(11)	124(11)	103(10)	-9(9)	61(9)	8(10)
C20	265(13)	125(11)	197(13)	-8(11)	-7(11)	62(10)
C21	227(12)	155(11)	180(12)	20(11)	-40(11)	-9(10)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 11 CCDC 110868 PJC6.

	x	y	z	U_{iso}
H0	5526(15)	4525(15)	3044(12)	16(6)
H1	5859(13)	5690(13)	2397(13)	14(6)
H2	6404(12)	3596(12)	2500	9(7)
H3	6819(14)	5806(15)	915(13)	6(5)
H4	6428(15)	4326(15)	690(13)	16(7)
H5	7428(13)	3365(14)	1368(12)	8(5)
H8	6791(13)	6400(14)	3527(13)	13(6)
H9	6308(16)	5142(15)	4293(14)	21(6)
H10	7315(14)	3954(15)	4016(13)	11(6)
H11A	8001(16)	2913(14)	2937(13)	11(6)
H11B	8735(18)	2939(18)	3372(17)	35(8)
H11C	8819(17)	2703(18)	2521(17)	41(8)
H12A	9929(18)	4970(20)	2570(16)	36(7)
H12B	10090(20)	4170(20)	2233(19)	52(10)
H12C	10070(20)	4210(20)	3020(20)	58(11)
H13A	9428(18)	6997(19)	1860(16)	39(8)
H13B	9595(16)	6057(16)	1738(15)	24(7)
H13C	9584(16)	6422(16)	2539(15)	29(7)
H14A	7030(20)	7093(19)	1901(17)	42(8)
H14B	7747(17)	7493(16)	1617(16)	30(7)
H14C	7622(18)	7635(19)	2416(18)	45(8)
H16	5254(16)	6425(15)	3931(13)	13(6)
H17	4810(12)	4987(12)	4340(11)	1(5)
H18	3424(13)	4664(15)	3775(12)	5(5)
H20A	3514(16)	8505(16)	3058(15)	20(7)
H20B	2890(20)	8063(19)	2606(19)	50(9)
H20C	3591(18)	8641(18)	2270(17)	39(8)
H21A	5429(18)	8059(18)	2155(16)	33(8)
H21B	5318(16)	8214(17)	3017(15)	26(7)
H21C	5715(17)	7370(17)	2717(15)	33(8)

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Principal mean square atomic displacements U

0.0104	0.0075	0.0059	Zr1
0.0136	0.0074	0.0055	Zr2
0.0126	0.0107	0.0083	Si1
0.0131	0.0100	0.0084	Si2
0.0167	0.0110	0.0083	Si3
0.0151	0.0114	0.0050	C1
0.0158	0.0121	0.0026	C2
0.0149	0.0127	0.0046	C3
0.0203	0.0103	0.0045	C4
0.0184	0.0099	0.0064	C5
0.0140	0.0105	0.0041	C6
0.0141	0.0108	0.0047	C7
0.0179	0.0140	0.0046	C8
0.0201	0.0097	0.0050	C9
0.0184	0.0116	0.0047	C10
0.0177	0.0159	0.0125	C11
0.0240	0.0204	0.0132	C12
0.0206	0.0143	0.0105	C13
0.0204	0.0184	0.0130	C14
0.0190	0.0127	0.0039	C15
0.0195	0.0148	0.0046	C16
0.0249	0.0100	0.0032	C17
0.0189	0.0126	0.0058	C18
0.0179	0.0129	0.0053	C19
0.0290	0.0196	0.0101	C20
0.0253	0.0167	0.0141	C21